

# Bushes of normal modes - new dynamical objects in nonlinear mechanical systems with discrete symmetry

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## Abstract

Bushes of normal modes represent exact mathematical objects describing specific dynamical regimes in nonlinear mechanical systems with point or space symmetry. In the present paper, we outline the bush theory and illustrate it with some bushes of small dimensions in octahedral mechanical structures.

## 1 Introduction

A new concept, “bushes of normal modes,” was introduced for nonlinear mechanical systems with discrete symmetry in [1, 2]. A given bush represents a certain superposition of the modes associated with different irreducible representations (irreps) of the symmetry group  $G$  of the mechanical system in equilibrium. The coefficients of this superposition are time-dependent functions for which the exact ordinary differential equations can be obtained. In this sense, the bush can be considered as a dynamical object whose dimensionality is frequently less than that of the original mechanical system. The following propositions were justified in previous papers [1, 2, 3]:

1. A certain subgroup  $G_D$  of the symmetry group  $G$  corresponds to a given bush, and this bush can be excited by imposing the appropriate initial conditions with the above symmetry group  $G_D \subset G$ .
2. Each mode belonging to the bush possesses its own symmetry group which is greater than or equal to the group  $G_D$  of the whole bush.
3. In spite of evolving mode amplitudes, the complete collection of modes in the given bush is preserved in time and, in this sense, the bush can be considered as a geometrical object.
4. The energy of the initial excitation is trapped in the bush, i.e. it cannot spread to the modes which do not belong to the bush, because of the symmetry restrictions.
5. As an indivisible nonlinear object, the bush exists because of force interactions between the modes contained in it.
6. Taking into account the concrete type of interactions between particles of the considered mechanical system can only reduce the dimension of the given bush.

7. The extension of the bush can be realized as a result of the loss of its stability which is accompanied by spontaneous breaking of the bush symmetry (dynamical analog of phase transition).

The special group-theoretical methods for finding bushes of modes are discussed in [3, 4]. The computer implementation of these methods [5] (see also [6]) allowed us to find bushes of modes for wide classes of mechanical systems with discrete symmetry. In particular, “irreducible” bushes of vibrational modes and symmetry determined similar non-linear normal modes for all  $N$ -particle mechanical systems with the symmetry of any of the 230 space groups were found in [4]. The bushes of vibrational modes of small dimensions were found and classified into universality classes for all mechanical systems with point groups of crystallographic symmetry in [7].

## 2 Outline of the bush theory

We consider classical Hamiltonian systems of  $N$  mass points moving near the single equilibrium state which can be characterized by a certain point or space symmetry group  $G$ . Let the  $3 \times N$ -dimensional vector,

$$\mathbf{X}(t) = (\mathbf{x}_1(t), \mathbf{x}_2(t), \dots, \mathbf{x}_N(t)), \quad (1)$$

describe the displacements  $\mathbf{x}_i(t)$  of all particles of our mechanical system from their equilibrium positions. (Here we denote by the three-dimensional vector  $\mathbf{x}_i$  the displacement of the  $i$ -th particle along the  $X$ ,  $Y$  and  $Z$  axes).

The vector  $\mathbf{X}(t)$  can be written as a superposition of all basis vectors  $\varphi_i^{(j)}$  of the irreducible representations  $\Gamma_j$  of the above mentioned symmetry group  $G$ :

$$\mathbf{X}(t) = \sum_{j,i} \mu_i^{(j)}(t) \varphi_i^{(j)}. \quad (2)$$

The coefficients  $\mu_i^{(j)}(t)$  of this superposition depend on time  $t$ , while the  $3 \times N$ -dimensional time-independent vectors  $\varphi_i^{(j)}$  are determined the specific patterns of displacements of all particles of our mechanical system.

Note that individual components of the basis vectors  $\varphi_i^{(j)}$  are often called “symmetry-adapted coordinates”. In particular, they can be normal coordinates. Hereafter, the term, “mode,” means an arbitrary superposition of basis vectors corresponding to a given irrep  $\Gamma_j$ . As a result of this definition, every term  $\mu_i^{(j)}(t) \varphi_i^{(j)}$  in the right hand side of Eq.(2) is also a mode of the irrep  $\Gamma_j$ . Sometimes, for brevity, we will refer to  $\mu_i^{(j)}(t)$  as a mode, but a reader must imagine that this time-dependent coefficient is multiplied by the appropriate  $3 \times N$ -dimensional vector  $\varphi_i^{(j)}$  to give the mode in the exact sense. We can also speak about *vibrational* modes because only such type of symmetry-adapted (normal) modes are considered in the present paper.

Every dynamical regime of the considered mechanical system can be described by the appropriate time-dependent vector  $\mathbf{X}(t)$  which determines a definite instantaneous configuration of the system. On the other hand, each instantaneous configuration possesses a certain symmetry group  $G_D$  (in particular, this group may be trivial:  $G_D = 1$ ) which is a subgroup of the symmetry group  $G$  of the system in equilibrium ( $G_D \subseteq G$ ). Moreover, we can also ascribe a certain symmetry group to each basis vector  $\varphi_i^{(j)}$  and to each mode corresponding to a given irrep  $\Gamma_j$  (remember that a mode is a superposition

of such vectors!), because the definite instantaneous configurations correspond to them. The group  $G_D$  contains all symmetry elements of group  $G$  whose action does not change this configuration.

Let us introduce, as it is usual in group theory, the operators  $\hat{g}$  associated with elements  $g$  of group  $G$  ( $g \in G$ ) which act on  $3 \times N$ -dimensional vectors  $\mathbf{X}(t)$ .<sup>1</sup> All elements  $g \in G$  for which

$$\hat{g}\mathbf{X}(t) = \mathbf{X}(t) \quad (3)$$

form a certain subgroup  $G_D \subseteq G$ , and a complete set of the above operators  $\hat{g}$  ( $\forall g \in G_D$ ) represents the group  $\widehat{G}_D$ .

It can be shown that the symmetry group  $G_D$  is preserved in time in the sense that its elements *cannot disappear* during time evolution. Actually, this property is a consequence of the principle of determinism in classical mechanics.<sup>2</sup> Thus, the equation  $\hat{g}\mathbf{X}(t) = \mathbf{X}(t)$  ( $g \in G_D$ ), or, formally,

$$\widehat{G}_D\mathbf{X}(t) = \mathbf{X}(t) \quad (4)$$

is valid for every time  $t$ . As a consequence, we can classify the different dynamical regimes in our nonlinear dynamical system, described by the vectors  $\mathbf{X}(t)$  from Eqs.(1,2), with the aid of *symmetry groups* corresponding to them.

Using Eq.(4), we can obtain the similar *invariance conditions* for each individual irrep  $\Gamma_j$  of the group  $G$  (see details in [3]):

$$(\Gamma_j \downarrow G_D)\boldsymbol{\mu}_j = \boldsymbol{\mu}_j. \quad (5)$$

Here  $(\Gamma_j \downarrow G_D)$  is a restriction of the irrep  $\Gamma_j$  to the subgroup  $G_D$  of the group  $G$ , and  $\boldsymbol{\mu}_j = (\mu_1^{(j)}, \dots, \mu_{n_j}^{(j)})$  is an *invariant vector* of  $\Gamma_j$  ( $n_j$  is the dimension of this irrep).

To find all modes contributing to a given dynamical regime with symmetry group  $G_D$ , i.e., for the vector  $\mathbf{X}(t)$  from Eq.(2), we must solve linear algebraic equations (5) for each irrep  $\Gamma_j$  of the group  $G$ . As a result of this procedure, the invariant vector  $\boldsymbol{\mu}_j$  for some irreps  $\Gamma_j$  can turn out to be equal to zero. Such irreps do not contribute to the considered dynamical regime. On the other hand, some nonzero invariant vectors  $\boldsymbol{\mu}_j$  for multidimensional irreps may be of a very specific form because of definite relations between their components (for example, certain components can be equal to each other, or differ only by sign).

Actually, Eq.(5) can be considered as a source of certain selection rules for spreading excitation from the root mode to a number of other (secondary) modes. Indeed, if a certain mode with the symmetry group  $G_D$  is excited at the initial instant (we call it the “root” mode), this group determines the symmetry of the whole bush. The condition that the appropriate dynamical regime  $\mathbf{X}(t)$  must be invariant under the action of the above group  $G_D$  leads to Eq.(4) and then to Eq.(5). If the vector  $\boldsymbol{\mu}_j$  for a given irrep  $\Gamma_j$  proves to be a zero vector, then there are no modes belonging to this irrep which contribute to  $\mathbf{X}(t)$ , i.e., the initial excitation *cannot spread* from the root mode to the secondary modes associated with the irrep  $\Gamma_j$ .

Note that basis vectors associated with a given irrep  $\Gamma_j$  in Eq.(2) turn out to be equal to zero when this irrep is not contained in the decomposition of the full vibrational irrep  $\Gamma$  into its irreducible parts  $\Gamma_j$ . This is a source of the additional selection rules which reduce the number of possible vibrational modes in the considered bush. Trying every

<sup>1</sup>The symmetry elements  $g \in G$  act on the vectors of three-dimensional Euclidean space.

<sup>2</sup>The phenomenon of spontaneous breaking of symmetry of a given dynamical regime will be considered in the next section.

irrep  $\Gamma_j$  in Eq.(5) and analyzing the above mentioned decomposition of the vibrational representation  $\Gamma$ , we obtain the whole bush of modes with the symmetry group  $G_D$  in the explicit form.

Let us return to Eq.(2). We speak about geometrical aspects of the bush theory when concentrate our attention on basis vectors  $\varphi_i^{(j)}$ , and we speak about dynamical aspects of this theory when we focus on time-dependent coefficients  $\mu_i^{(j)}(t)$ , which will be also called “modes”.

If interactions between the particles of our mechanical system are known, *exact* dynamical equations describing the time evolution of a given bush can be written.

Two types of interactions between modes in nonlinear Hamiltonian system are discussed in [3], namely, *force* interactions and *parametric* interactions. We can illustrate the difference between these types of modal interactions using a simple example.

Let us consider two different linear oscillators whose coupling is described by only one anharmonic term,  $U = -\gamma\mu_1^2\mu_2$ , in the potential energy. Dynamical equations for this system can be written as follows:

$$\ddot{\mu}_1 + \omega_1^2\mu_1 = 2\gamma\mu_1\mu_2, \quad (6)$$

$$\ddot{\mu}_2 + \omega_2^2\mu_2 = \gamma\mu_1^2. \quad (7)$$

Here  $\gamma$  is an arbitrary constant characterizing the strength of the interaction of the oscillators. We can suppose that Eqs.(6,7) describe the dynamics of two modes  $\mu_1(t)$  and  $\mu_2(t)$  in a certain mechanical system.

An essential disparity between modes  $\mu_1(t)$  and  $\mu_2(t)$  can be seen from the above equations. Indeed, if we excite the mode  $\mu_1(t)$  at the initial instant ( $\mu_1(t_0) \neq 0$ ), the mode  $\mu_2(t)$  cannot be equal to zero (even if it was zero at  $t = t_0$ !) because a *nonzero force*  $-\frac{\partial U}{\partial \mu_2} = \gamma\mu_1^2$  appears in the right hand side of Eq.(7) since  $\mu_1(t) \neq 0$ . In other words, the dynamical regime  $\mu_1(t) \neq 0, \mu_2(t) \equiv 0$  cannot exist because of the contradiction with Eq.(7). Unlike this, the dynamical regime  $\mu_2(t) \neq 0, \mu_1(t) \equiv 0$  can exist because such a condition does not contradict equations (6) and (7). We can say that now there is no force in the right hand side of Eq.(7) because  $\frac{\partial U}{\partial \mu_2} \equiv 0$  as a consequence of the identity  $\mu_1(t) \equiv 0$ .

In the last case, the dynamical regime of the system (6,7) represents a harmonic oscillation only of the second variable:

$$\mu_2(t) = A \cos(\omega_2 t + \delta), \quad (8)$$

where  $A$  and  $\delta$  are two arbitrary constants.

Thus, there is *force* action from the mode  $\mu_1(t)$  on the mode  $\mu_2(t)$ , but not vice versa. We proved in [3] that such a situation can be realized only in the case where the symmetry group of the mode  $\mu_1(t)$  is less than or equal to that of the mode  $\mu_2(t)$ .<sup>3</sup>

Nevertheless, the mode  $\mu_2(t)$  can excite the mode  $\mu_1(t)$  under certain circumstances. Indeed, substituting the solution (8) of Eq.(7) into Eq.(6), we obtain

$$\ddot{\mu}_1(t) + [\omega_1^2 - 2A\gamma \cos(\omega_2 t + \delta)] \mu_1 = 0. \quad (9)$$

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<sup>3</sup>Remember, that speaking about a mode we must take into account that our time-dependent coefficient is multiplied by the appropriate basis vector of a certain irrep of the group  $G$ , and namely this vector determines the symmetry group of the considered mode.

By means of simple algebraic transformations this equation can be converted to the Mathieu equation in its standard form:

$$z'' + [a - 2q \cos(2\tau)] z = 0, \quad (10)$$

where  $z = z(\tau)$ . But in the  $(a - q)$  plane of the Mathieu equation (10) there exist domains of stable and unstable movement. If pertinent parameters  $(\omega_1, \omega_2, \gamma)$  of our dynamical system (6,7) have values such that corresponding parameters  $a$  and  $q$  of Eq.(10) get into an unstable domain, then the nonzero function  $z(\tau)$  and, therefore, the mode  $\mu_1(t)$  appears. In other words, the initial dynamical regime  $\mu_1(t) \equiv 0, \mu_2(t) \not\equiv 0$  loses its stability, and a new dynamical regime  $\mu_1(t) \not\equiv 0, \mu_2(t) \not\equiv 0$  arise *spontaneously* for definite values of the parameters of Eqs.(6,7). Since this phenomenon is similar to the well-known parametric resonance, we can speak, in such a case, about *parametric action* from the mode  $\mu_2(t)$  on the mode  $\mu_1(t)$ .

The characteristic property of the parametric interaction is that the appropriate force  $(-\frac{\partial U}{\partial \mu_1} = 2\gamma\mu_1\mu_2$ , in our case) vanishes when the mode ( $\mu_1$ , in our case), on which this force acts, becomes zero. The following important result was proved in [3]: the mode of lower symmetry acts on the mode of higher symmetry by *force* interaction, while the mode of higher symmetry can act on the mode of lower symmetry only *parametrically*. Consequently, if the parametric excitation of a certain mode does take place, this phenomenon must be by necessity be accompanied by *spontaneous breaking* of symmetry of the mechanical system vibrational state.

Thus, the initially excited dynamical regime can lose its stability because of parametric interactions with some zero modes and, as a result, can transform spontaneously into another dynamical regime, described by a greater number of dynamical variables, with appropriate lowering of symmetry. Obviously, we may treat such phenomenon as a dynamical analog of a phase transition.

### 3 Examples of bushes of vibrational modes

We consider a mechanical system of six mass points (particles) whose interactions are described by a pair isotropic potential  $u(r)$  where  $r$  is the distance between two particles. We suppose that in the *equilibrium state* these particles form a regular octahedron with edge  $a_0$  which can be imagined in the following way. Let us introduce a Cartesian coordinate system. Four particles of the above octahedron lie in the  $XY$  plane and form a square with edge  $a_0$ . Two other particles lie on  $Z$  axis and we will speak about the “top particle” and the “bottom particle” with respect to the direction of the  $Z$  axis. Obviously, the distance between each of these two particles and any of the four particles in the  $XY$  plane is equal to  $a_0$ .

The point symmetry group of the octahedral equilibrium configuration is  $O_h$  and all bushes of vibrational modes in the considered system are described by the certain subgroups  $G_D$  of this parent group. In the present paper, we consider only three bushes<sup>4</sup>  $B1[O_h]$ ,  $B2[D_{4h}]$  and  $B4[C_{4v}]$  (the complete list includes 18 different by symmetry bushes of vibrational modes whose dimensions vary from 1 to 12). The symmetry groups of the above bushes are connected with each other by the following group-subgroup relation:  $C_{4v} \subset D_{4h} \subset O_h$ .

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<sup>4</sup>We write the symmetry group  $G_D$  of the bush in square brackets next to its symbol.

The geometrical forms of our mechanical system in the *vibrational state*, corresponding to these bushes, can be revealed from the appropriate symmetry groups  $G_D$ .

The one-dimensional bush  $B1[O_h]$  consists of only one (“breathing”) mode. This nonlinear dynamical regime  $\mathbf{X}(t) = \mu_1^{(1)}(t)\boldsymbol{\varphi}_1^{(1)}$  describes evolution of a regular octahedron whose edges  $a = a(t)$  periodically change in time.

The two-dimensional bush  $B2[D_{4h}]$  describes a dynamical regime with two degrees of freedom:  $\mathbf{X}(t) = \mu_1^{(1)}(t)\boldsymbol{\varphi}_1^{(1)} + \mu_1^{(5)}(t)\boldsymbol{\varphi}_1^{(5)}$ . The symmetry group  $G_D = D_{4h}$  of this bush contains the 4-fold axis coinciding with the  $Z$  coordinate axis and the mirror plane coinciding with the  $XY$  plane. This symmetry group restricts essentially the form of the polyhedron describing our mechanical system in the vibrational state. Indeed, the presence of the 4-fold axis demands that the quadrangle in the  $XY$  plane be a square. Because of the same reason, the four edges connecting the particles in the  $XY$  plane (vertices of the above square) with the top particle lying on  $Z$  axis must be of the same length which we denote by  $b(t)$ .

Similarly, let the length of the edges connecting the bottom particle on the  $Z$  axis with any of the 4 particles in the  $XY$  plane be denoted by  $c(t)$ . In our present case of the bush  $B2[D_{4h}]$ ,  $b(t) = c(t)$  for any time  $t$  because of the presence of the horizontal mirror plane in the group  $G_D = D_{4h}$ . But for the three-dimensional bush  $B4[C_{4v}]$ , described by  $\mathbf{X}(t) = \mu_1^{(1)}(t)\boldsymbol{\varphi}_1^{(1)} + \mu_1^{(5)}(t)\boldsymbol{\varphi}_1^{(5)} + \mu_3^{(10)}(t)\boldsymbol{\varphi}_3^{(10)}$ , this mirror plane is absent and, therefore,  $b(t) \neq c(t)$ .

Let us also introduce two heights,  $h_1(t)$  and  $h_2(t)$ , corresponding to the perpendiculars dropped, respectively, from the top and bottom vertices of our polyhedron in the  $XY$  plane. Now we can write the dynamical equations of the above bushes in terms of pure geometrical variables  $a(t)$ ,  $b(t)$ ,  $c(t)$ ,  $h_1(t)$  and  $h_2(t)$ .

We choose  $a(t)$  and  $h(t) \equiv h_1(t) \equiv h_2(t)$  as dynamical variables for describing the two-dimensional bush  $B2[D_{4h}]$  and  $a(t)$ ,  $h_1(t)$  and  $h_2(t)$  as dynamical variables for describing the three-dimensional bush  $B4[C_{4v}]$ . Using these variables we can write down the potential energy for our bushes of vibrational modes as follows:

$$\begin{aligned} B1[O_h] &: V_{B1}(a) = 12u(a) + 3u(\sqrt{2}a), \\ B2[D_{4h}] &: V_{B2}(a, h) = 4u(a) + 2u(\sqrt{2}a) + 8u\left(\sqrt{h^2 + \frac{a^2}{2}}\right) + u(2h), \\ B4[C_{4v}] &: V_{B4}(a, h_1, h_2) = 4u(a) + 2u(\sqrt{2}a) + 4u(b) + 4u(c) + u(h_1 + h_2), \end{aligned}$$

$$\text{where } b = \sqrt{\frac{a^2}{2} + \left(\frac{5}{4}h_1 - \frac{1}{4}h_2\right)^2}, \quad c = \sqrt{\frac{a^2}{2} + \left(\frac{5}{4}h_2 - \frac{1}{4}h_1\right)^2}.$$

Then with the aid of the Lagrange method, we can obtain the following dynamical equations for the above bushes of vibrational modes:

$$\begin{aligned} B1[O_h] : \quad & \ddot{a} = -4u'(a) - \sqrt{2}u'(\sqrt{2}a); \\ B2[D_{4h}] : \quad & \ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - 2u'(b)\frac{a}{b}, \\ & \ddot{h} = -4u'(b)\frac{h}{b} - u'(2h); \\ B4[C_{4v}] : \quad & \ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - u'(b)\frac{a}{b} - u'(c)\frac{a}{c}, \\ & \ddot{h}_1 = -u'(b)\frac{5h_1 - h_2}{b} - u'(h_1 + h_2), \\ & \ddot{h}_2 = -u'(c)\frac{5h_2 - h_1}{c} - u'(h_1 + h_2). \end{aligned} \tag{11}$$

Thus, we obtain the dynamical equations of our bushes of vibrational modes in terms of variables with explicit geometrical sense. Each bush describes a certain nonlinear

dynamical regime corresponding to such a vibrational state of the considered mechanical system, that at any fixed time the configuration of this system is represented by a definite polyhedron with symmetry group  $G_D$  of a given bush.

We can write dynamical equations for the above bushes in terms of vibrational modes as well. In spite of the more complicated form, these equations turn out to be more useful for the bush theory, since they allow us to decompose the appropriate nonlinear dynamical regimes into modes of different importance for the case of small oscillations – root modes and secondary modes of different orders [3]. As an example, we write below the dynamical equations for the bush  $B4[C_{4v}]$  in terms of its three modes,  $\mu_3^{(10)}(t) \equiv \gamma(t)$  (root mode),  $\mu_1^{(1)}(t) \equiv \mu(t)$ ,  $\mu_1^{(5)}(t) \equiv \nu(t)$  (secondary modes):

$$\begin{aligned}\ddot{\mu} = & -\frac{1}{6}(4\sqrt{2}u'(a) + 4u'(\sqrt{2}a) + 2u'(h_1 + h_2) + \frac{u'(b)}{b}(2\sqrt{2}a + 5h_1 - h_2) + \\ & \frac{u'(c)}{c}(2\sqrt{2}a + 5h_2 - h_1)), \\ \ddot{\nu} = & -\frac{1}{6}(2\sqrt{2}u'(a) + 2u'(\sqrt{2}a) - 2u'(h_1 + h_2) + \frac{u'(b)}{b}(\sqrt{2}a - 5h_1 + h_2) + \\ & \frac{u'(c)}{c}(\sqrt{2}a - 5h_2 + h_1)), \\ \ddot{\gamma} = & \frac{1}{4} \left( u'(b) \frac{5h_1 - h_2}{b} - u'(c) \frac{5h_2 - h_1}{c} \right).\end{aligned}$$

Here

$$\begin{aligned}a &= \sqrt{2}(r_0 + \mu + \nu); b = \sqrt{(r_0 + \mu + \nu)^2 + (r_0 + \mu - 2\nu - 3\gamma)^2}; \\ c &= \sqrt{(r_0 + \mu + \nu)^2 + (r_0 + \mu - 2\nu + 3\gamma)^2}; \\ h_1 &= r_0 + \mu - 2\nu - 2\gamma; h_2 = r_0 + \mu - 2\nu + 2\gamma; r_0 = \frac{a_0}{\sqrt{2}}.\end{aligned}$$

In the previous section, the problem of existence of bushes of vibrational modes was studied by group-theoretical methods only. In contrast to this, examination of the stability of the bushes depends essentially on the concrete type of interactions in the considered system, and we suppose that they can be described by a Lennard-Jones potential. Then the bush stability will be analyzed with the aid of numerical methods.

Let us excite a given bush  $B[G_D]$  with the aid of the following *initial condition*. Note that the root mode of each of the above considered bushes is determined by a *single* time-dependent coefficient  $\mu_i^{(j)}(t)$  whose initial value at  $t = t_0$  we will denote by the symbol  $\mu_0$  ( $\mu_0 \equiv \mu_i^{(j)}(t_0)$ ). At the initial instant  $t = t_0$ , we fix the coordinates of all particles of the mechanical system in such a way that their *displacements* correspond to the appropriate root mode with amplitude  $\mu_0$ , while their velocities are equal to *zero*. Namely this choice of initial conditions determines the *way* of excitation of a given bush.

Using these initial conditions we solve numerically the exact dynamical equations of the considered mechanical system with 18 degrees of freedom, and analyze the set of nonzero modes  $\mu_i^{(j)}(t)$  in the decomposition (2) of the vector  $\mathbf{X}(t)$  obtained as a result of this solving. Then we gradually increase the value  $\mu_0$  and repeat the procedure just described until the number of nonzero modes  $\mu_i^{(j)}(t)$ , at some value  $\mu_0 = R$ , becomes larger than that of the bush  $B[G_D]$ . We will refer to  $R$  as the *threshold* of stability of the given bush. Obviously, in such a way we obtain the upper boundary of the first stability region of  $B[G_D]$  in one-dimensional space of all possible values  $\mu_0$  ( $0 < \mu_0 \leq R$ ).<sup>5</sup>

<sup>5</sup>Note that we do not study the *other* possible regions of stability of the given bush  $B[G_D]$  in the present paper.

For  $\mu_0 > R$  a new bush  $\tilde{B}[\widetilde{G}_D]$ , including the old bush  $B[G_D]$ , appears and its symmetry  $\widetilde{G}_D$  is *lower* than that of this old bush ( $\widetilde{G}_D \subset G_D$ ), because all modes with symmetry higher than or equal to  $G_D$  are already contained in  $B[G_D]$ .

Thus, the loss of stability of a given bush is accompanied by the spontaneous breaking of symmetry of the initially excited dynamical regime, described by this bush. We already discussed this phenomenon in Sec.2 and concluded that its cause is analogous to that of this parametric resonance.

We can also say this in other words. A given bush  $B[G_D]$  represents a certain dynamical regime in the considered mechanical system. Its modes interact with other modes which do not belong to  $B[G_D]$ , but these interactions must be of parametric (not force!) type only. For the appropriate initial conditions we can get into a region of unstable movement. As a result, some new modes are excited which were forbidden by principle of determinism of classical mechanics. Then we can speak about the loss of stability of the original bush  $B[G_D]$  and its transformation into a larger bush  $\tilde{B}[\widetilde{G}_D]$  with ( $\widetilde{G}_D \subset G_D$ ).

The Lennard-Jones potential can be written in the form,

$$u(r) = \frac{A}{r^{12}} - \frac{B}{r^6}, \quad (12)$$

with  $A = B = 1$  (because of the appropriate scaling transformation of space and time variables). Our numerical experiments give the following values of the threshold  $R$  for the above considered bushes:

$$R[B1] = 0.001, \quad R[B2] = 0.009, \quad R[B4] = 0.003. \quad (13)$$

Note that these values of  $R$  are finite but very small in comparison with the edge  $a_0 = 1.117$  of our octahedral structure in equilibrium. Displacements of particles corresponding to the thresholds (13) can be obtained by dividing these three values of  $R$  by the numbers  $\sqrt{6}$ ,  $\sqrt{12}$ ,  $\sqrt{12}$ , respectively. We want to note in this connection, that all octahedral molecules, known to us at the present time, possess an atom in the center of the octahedron. This fact suggests that the stability of such structures can be greater than that of the mechanical system considered up to this point. Taking into account this hint, we examined bush stability for the mechanical structure with the particle in the center of the octahedron, supposing that this additional (seventh) particle is described by the Lennard-Jones potential different from that for six peripheral particles. Namely, we assume that  $A = 1$ , but  $B > 1$  in Eq.(12). Such an assumption provides us a possibility of making the attractive part of the potential of the centered particle greater than that of peripheral atoms in spite of the same repulsive part.

For such a centered structure the threshold values  $R$  can be essentially greater than those for the structure without the particle in the center of the octahedron. Indeed, we obtained that  $R[B1] = 1.010$ ,  $R[B2] = 0.011$ ,  $R[B4] = 0.118$  for  $B = 5.5$ . Note that the dependence of the threshold  $R$  on the value  $B$  is essentially different for different bushes and can be nonmonotonic.

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